AC transport with reservoirs of finite width

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Abstract

The linear response conductance coefficients are calculated in the scattering approach at finite frequency, damping and magnetic field for a microstructure in which the reservoirs are modeled as quantum wire leads of infinite length but finite width. Independently of frequency, inelastic scattering causes subbands with large group velocity to contribute more strongly to the conductance than channels of comparable transmission but slower propagation. At finite frequency and magnetic fields, additional correction terms appear, some of which are sensitive to the phase of the S matrix.

The Landauer-Büttiker formula [1] for the low-temperature, linear-response DC conductance coefficients of a small conductor requires only the knowledge of the quantum mechanical transmission coefficients, i.e. absolute values of S-matrix elements. The S-matrix in turn appears because one necessarily has to consider the system as being open, i.e. having a continuous spectrum. With discrete levels, no dissipative response is possible. One often uses a model in which the sample is connected to the outside world by straight quantum wires of infinte length [2].

Here, we want to study the linear conductance of such an open system under an AC perturbation. The limiting case of infinitely broad reservoirs and no damping has been considered previously, [3], yielding an *admittance matrix* for $n \neq l$

$$g_{nl}(\omega) = \frac{e^2}{h} \int dE \, \frac{f(E) - f(E + \hbar\omega)}{\hbar\omega} \, \mathrm{Tr}\left\{ S^{\dagger}_{nl}(E) \, S_{nl}(E + \hbar\omega) \right\} . \tag{1}$$

Here, n and l label the leads so that $\langle I_n(\omega) \rangle = \sum_l g_{nl}(\omega) \, V_l(\omega)$, and the trace extends over subbands. An apparent conflit has been noted [4] between the widespread use of Landauer-type formulas even in systems that are one-dimensional at infinity, and the requirement that the reservoirs have to be much wider than the sample itself to permit equilibration.

We provide an answer to this open question by considering the linear response of a system with quantum wire leads, including an inelastic scattering rate in the equation of motion.

Electron-electron interactions are assumed to be absent in the reservoir region. An external uniform magnetic field B is taken into account.

Consider a system under the influence of an external perturbation, $H = H_0 + H_1$, where H_0 is the unperturbed time-independent Hamiltonian and (in the interaction picture)

$$H_{1I}(t) \equiv -e \int n_I(\mathbf{x}, t)\, \Phi(\mathbf{x})\, d\mathbf{x} \equiv e^{i\omega t}\, F_I(t). \tag{2}$$

Here, $n_I(t)$ is the number density operator. The assumption that a static potential Φ can describe the field distribution amounts to neglecting the rotational part of the time-varying electric field. The fact that the resulting perturbation (which must also contain the self-consistent induced fields) just adds to the original Hamiltonian H_0 is a consequence of the linear response approximation. The expectation value of the current density is $\langle j(\mathbf{x},\, t)\rangle = Tr\, \rho(t)\, j$, where we use the *linear approximation* in the von-Neumann equation for the density matrix,

$$\frac{\partial}{\partial t}\rho_I(t) = \frac{1}{i\hbar}\, [H_{1I}(t), \rho_0] - \gamma\, \{\rho_I(t) - \rho_0\}\,. \tag{3}$$

Here ρ_0 is the equilibrium density and γ is an *inelastic relaxation rate* [5, 6]. To solve this in the basis of many-body eigenstates $|\alpha\rangle$ of H_0 with energy ϵ_α, one needs the matrix elements of Eq. (2). Using the continuity equation, $\dot{n}_I(\mathbf{x}, t) = -\nabla \cdot \mathbf{j}_I(\mathbf{x}, t)$, one can perform an integration by parts as in Ref. [7], yielding

$$\begin{aligned} \langle\alpha|F_I(t)|\beta\rangle \;&=\; \frac{ie\hbar}{\epsilon_\alpha - \epsilon_\beta} \Bigg\{ \int\limits_{\partial\mathcal{A}} \langle\alpha|\mathbf{j}_I(\mathbf{x}, t)|\beta\rangle\, \Phi(\mathbf{x})\, d\mathbf{x} \\ &\quad - \int\limits_{\mathcal{A}} \Phi(\mathbf{x})\, \nabla \cdot \langle\alpha|\mathbf{j}_I(\mathbf{x}, t)|\beta\rangle\, d\mathbf{x} \Bigg\}. \end{aligned} \tag{4}$$

Here, $\mathbf{j}_I$ is the current operator associated with H_0, containing at most a static vector potential if the Landau gauge is chosen in each lead[2].

With this procedure, we have traded the infinite integration domain of Eq. (2) for a finite domain $\mathcal{A}$. The price that was paid is the additional boundary integral over $\partial\mathcal{A}$. At $\omega = \gamma = 0$, the contribution of the bulk term is known to vanish [2]. Its significance at finite frequency as compared to the surface term is not addressed in Ref. [3], but it has been stated[8] that it should be negligible at small frequencies, when one is in the quasi-stationary regime, $\boldsymbol{\nabla}\mathbf{j} \approx 0$. However, an estimate of the conditions for this regime is not available in the literature.

Using $\langle\alpha|\rho|\beta\rangle$, the current response becomes

$$\langle\mathbf{j}(\mathbf{x},\, t)\rangle = \mathbf{j}_0(\mathbf{x}) - e^{i\omega t} \sum_{\alpha\beta} \frac{\langle\beta|\mathbf{j}_I(\mathbf{x},\, t)|\alpha\rangle\, \langle\alpha|F_I(t)|\beta\rangle}{\hbar\omega + \epsilon_\alpha - \epsilon_\beta + i\hbar\gamma}\, (P_\alpha - P_\beta). \tag{5}$$

Here, $\mathbf{j}_0(\mathbf{x})$ is the unperturbed equilibrium current, and $P_\alpha = \langle\alpha|\rho_0|\alpha\rangle$. The total current is the integral of Eq. (5) over the cross section of lead n. Furthermore, we only need the deviation from the equilibrium value, so that we bring the term involving $\mathbf{j}_0(\mathbf{x})$ to the lefthand side. The resulting induced current has the time dependence $e^{i\omega t}$, which we drop to get the corresponding Fourier component (which can still be a function of the distance x from the sample).

For the bulk term in Eq. (4), we can calculate the total current through all the leads,

$$\begin{aligned}\sum_n I_n^{\mathrm{bulk}} &= \int_{\mathcal{A}} \nabla \cdot \langle \mathbf{j}^{\mathrm{bulk}}(\mathbf{x}') - \mathbf{j}_0^{\mathrm{bulk}}(\mathbf{x}')\rangle d\mathbf{x}' \\ &= -\frac{ie^2}{\hbar} \sum_{\alpha\beta} \frac{P_\beta - P_\alpha}{\epsilon_\beta - \epsilon_\alpha - \hbar z}(\epsilon_\beta - \epsilon_\beta) \times \\ &\quad \int_{\mathcal{A}} \langle \beta | n(\mathbf{x}') | \alpha \rangle \, \Phi(\mathbf{x}) \, \langle \alpha | n(\mathbf{x}) | \beta \rangle \, d\mathbf{x}' \, d\mathbf{x}, \end{aligned} \tag{6}$$

where Gauss' theorem and the continuity equation were used. We henceforth abbreviate $z \equiv \omega - i\gamma$. To linear order in z, this can be expressed in terms of the Green's function, $G(E) = \sum_\alpha |\alpha\rangle\langle\alpha|/(E - \epsilon_\alpha)$, as

$$\sum_n I_n^{\mathrm{bulk}} = -ie^2 z \sum_\beta P_\beta \int_{\mathcal{A}} \Phi(\mathbf{x}) \, \langle \beta | n(\mathbf{x}') \, G(\epsilon_\beta) \, n(\mathbf{x}) + \mathrm{h.c.} \, |\beta\rangle \, d\mathbf{x}' \, d\mathbf{x}. \tag{7}$$

The similarity of this operator expression to the mean-field-like result of Ref. [4] [cf. Eq. (54) therein, summed over leads] leads us to identify this contribution with the internal response, which we have thus re-derived in an alternative way.

In the following we shall focus on the boundary term and find a generalization of the external response result of Ref. [4, 9]. The N mutually decoupled, straight infinite quantum wires leads at large distance from the sample are described by a non-interacting Hamiltonian H_{QW}. The many-body eigenstates $|\alpha\rangle$ of the full unperturbed system decompose into Slater determinants of single-particle eigenstates of H_{QW} in the asymptotic region, a complete set of which is given by the scattering states, ψ^l_{Eap} at energy E, consisting of an incoming wave in subband a of lead p, and of outgoing waves in all the subbands of all the leads l. Using local coordinates x, y parallel and transverse to the wire l, the energy-normalized quantum wire eigenfunctions are

$$\xi^l_{\pm a}(\mathbf{x}) \equiv \left| 2\pi \, \frac{dE^l_a}{dk} \right|^{-1/2} e^{i\mathrm{k}^l_{\pm a} x} \, \chi^l_{\mathrm{k}^l_{\pm a} a}(y). \tag{8}$$

Unless $B = 0$ in the leads, the transverse wavefunctions $\chi^l_{ka}(y)$ are also functions of the wavenumber $\mathrm{k}^l_{\pm a}(E)$. The $+$ ($-$) sign denotes propagation toward (away from) the sample. The scattering states in lead l then are

$$\psi^l_{Eap} \equiv \delta_{pl} \, \xi^l_{-a}(\mathbf{x}) + \sum_{a'} S_{lp,a'a} \, \xi^l_{+a'}. \tag{9}$$

Here, $S_{lp,a'a}$ is the S matrix element for scattering from subband a of lead p to subband a' of lead l. Bound states of the system do not enter in the completeness relation because of their exponential decay.

After making the transition to the single-particle scattering states, the boundary contribution to the current at a distance x along lead n from the sample takes the form

$$
\begin{aligned}
I_n(x) &= -ie^2\hbar \sum_{l=1}^{N} V_l \sum_{p,q=1}^{N} \sum_{a,b=0}^{\infty} \int_{-\infty}^{\infty} dE'\, dE\, \frac{f(E')-f(E)}{E-E'} \\
&\quad \times \frac{\langle \psi^l_{Eap} | J^l(x_{\mathcal{A}}) | \psi^l_{E'bq} \rangle \, \langle \psi^n_{E'bq} | J^n(x) | \psi^n_{Eap} \rangle}{E'-E-\hbar z}. \qquad (10)
\end{aligned}
$$

Here, J^l is the component of the single-particle current operator along lead l, integrated over the cross section at a distance $x_{\mathcal{A}}$ from the sample (determined by $\partial\mathcal{A}$). We use the convention that subscripts a or a' are always associated with a dependence on E, while b or b' labels functions of E'. If we now insert Eq. (9), then the last line in Eq. (10) contains a product of current matrix elements between quantum wire eigenfunctions at different energies, of the type considered in Ref. [7]. For brevity, we restrict ourselves to g_{nl} with $n \neq l$. In that case one can exploit the δ_{pl} in Eq. (9), as well as the unitarity relation $S^\dagger(E)\, S(E) = 1$. Furthermore, current matrix elements between counter-propagating waves such as $\langle \xi^l_{-a} | J^l | \xi^l_{+b} \rangle$ vanish as $\omega \to 0$. To linear order in ω, this leaves

$$
\begin{aligned}
g_{nl} &= -ie^2\hbar \sum_{a,b,a',b'=0}^{\infty} \int_{-\infty}^{\infty} dE'\, dE\, \frac{f(E')-f(E)}{E-E'} \\
&\quad \times \frac{1}{E'-E-\hbar z} \Big\{ \langle \xi^l_{-a} | J^l | \xi^l_{-b} \rangle \, \langle \xi^n_{+b'} | J^n | \xi^n_{+a'} \rangle \, S^*_{nl,b'b}\, S_{nl,a'a} \\
&\quad + \langle \xi^l_{+a'} | J^l | \xi^l_{+b'} \rangle \, \langle \xi^n_{-b} | J^n | \xi^n_{-a} \rangle \, S^*_{ln,a'a}\, S_{ln,b'b} \Big\} \qquad (11)
\end{aligned}
$$

The arguments on the current operators were left out, keeping in mind that the coordinates are $x_{\mathcal{A}}$ in leads l and x in lead n. Following Ref. [3], one of the energy integrals is done such that all terms multiplied by $f(E)$ are integrated over E', *vice versa* for terms multiplied by $f(E')$. Applying the residue theorem, the poles of the Fermi function then do not enter. If the first term in braces is integrated over E (E'), we close the contour by a large semicircle in the positive (negative) imaginary plane; for the second term in braces, the opposite contour is taken. With this choice, all the $e^{\pm ikx}$ factors in the wire eigenfunctions ξ yield exponential suppression along the return contour due to the imaginary part of k. Poles of S occur only in the negative energy plane, and in the positive plane for S^*. As a consequence, the above choice of contours always selects the half plane in which no poles of the S-matrix are enclosed. The contributions from the pole at $E' = E$ cancel due to the difference of Fermi functions, so that the only pole that remains is the one at $E' = E + \hbar z$. However, this pole is never enclosed for the second term in braces, so that the latter makes no contribution at all. We are thus left with

$$
\begin{aligned}
g_{nl} &= 2\pi\, e^2\hbar \sum_{a,b,a',b'=0}^{\infty} \int_{-\infty}^{\infty} dE\, \frac{f(E+\hbar z)-f(E)}{\hbar z} \\
&\quad \times \langle \xi^l_{-a} | J^l | \xi^l_{-b} \rangle \, \langle \xi^n_{+b'} | J^n | \xi^n_{+a'} \rangle \, S^*_{nl,b'b}\, S_{nl,a'a} \Big|_{E'=E+\hbar z}. \qquad (12)
\end{aligned}
$$

At $B = 0$, the transverse modes are orthogonal irrespective of energy, yielding immediately the requirement $a = b$, $a' = b'$. Consider these terms first, but at $B \neq 0$. Expand all wavenumbers around E, recalling that b labels functions of $E+\hbar z$, e.g.

$$\mathrm{k}^l_{-b}(E+\hbar z) \approx \mathrm{k}^l_{-b}(E) + q^l_{-a}, \quad q^l_{-a} \equiv \frac{z}{v^l_{g,-a}(E)}. \tag{13}$$

Here, we introduced the channel-specific group velocity $v^l_{g,\pm a}(E) \equiv (1/\hbar)\, dE^l_a(\mathrm{k}^l_{\pm a}(E))/dk$. Then first-order perturbation theory yields for the transverse channel eigenfunctions

$$\chi^l_{-b,E+\hbar z} = \chi^l_{-a} - \hbar\omega_c\, q^l_{-a} \sum_{a'\neq a} \chi^l_{-a'} \frac{\langle \chi^l_{-a'}|y'|\chi^l_{-a}\rangle}{E^l_{-a}(\mathrm{k}^l_{-a}(E)) - E^l_{-a'}(\mathrm{k}^l_{-a}(E))}, \tag{14}$$

where $\omega_c = eB/mc$. This can be used to evaluate the current matrix elements in Eq. (12) with the Landau gauge, where one needs $\langle \chi^l_{-a}|\chi^l_{-b}\rangle$, $\langle \chi^l_{-a}|y'|\chi^l_{-b}\rangle$ and $\langle \chi^n_{+b'}|\chi^n_{+a'}\rangle$, $\langle \chi^n_{+b'}|y|\chi^n_{+a'}\rangle$. To get explicit expressions, we specialize to *parabolic* quantum wires with the same dispersion relation in leads n and l,

$$E_a(k) = \frac{\hbar^2 k^2}{2m}\, \frac{\omega_0^2}{\omega_0^2+\omega_c^2} + \hbar\,\sqrt{\omega_0^2+\omega_c^2}\,\left(a+\frac{1}{2}\right). \tag{15}$$

The terms in Eq. (12) with $a=b$, $a'=b'$ then yield to linear order in z

$$\begin{aligned} g^{diag}_{nl} &= \frac{e^2}{h} \sum_{a,a'=0}^{\infty} \int_{-\infty}^{\infty} dE \left[-\frac{f(E+\hbar z)-f(E)}{\hbar z}\right] S^*_{nl,a'a}(E+\hbar z)\, S_{nl,a'a}(E) \\ &\quad \times e^{-i\,z\left(x/|v^n_{ga'}|+x_{\mathcal{A}}/|v^l_{ga}|\right)} \left\{1 + z\,\frac{m\omega_c^2}{2\hbar\omega_0^2}\left(\frac{1}{(k^n_{a'})^2} - \frac{1}{(k^l_a)^2}\right)\right. \\ &\qquad\qquad \left. \times \left(1+\frac{\omega_c^2}{\omega_0^2}\right)\left(1+\sqrt{1+\omega_c^2/\omega_0^2}\right)\right\} \end{aligned} \tag{16}$$

This reduces to Eq. (1) only if *both* $\omega_c = 0$ *and* one drops the exponential, which describes damped oscillations as a function of x and $x_{\mathcal{A}}$ since $z=\omega - i\,\gamma$. Note that $x_{\mathcal{A}}\,\gamma$ is the velocity that a particle must have in order to traverse the distance $x_{\mathcal{A}}$ before the inelastic damping becomes significant. Similarly, $x_{\mathcal{A}}\,\omega$ is the velocity that is required to traverse $x_{\mathcal{A}}$ in one oscillation period of the external field. If carriers can then enter and leave the sample region so fast that $z\,x/|v^n_{ga'}|$, $z\,x_{\mathcal{A}}/|v^l_{ga} \approx 0$, then the precise location of the current and voltage probes, which is given by x and $x_{\mathcal{A}}$, respectively, becomes irrelevant. In particular, channels exceeding the *cutoff* group velocity, $\max(x\gamma,\, x_{\mathcal{A}}\gamma)$, are essentially undamped in Eq. (16). Their number increases when the reservoirs are much wider than the sample region, in which case "slow" subbands typically have negligible transmission through the sample since coupling to the narrow sample requires large transverse momentum transfer. For narrow reservoirs, the transmission of such slow subbands can be appreciable, so that the deviation between Eqs. (1) and (16) can be significant even at $\omega = B = 0$.

We also find contributions from *off-diagonal terms* with $a \neq b$ or $a' \neq b'$ in Eq. (12), of which we list only one example[10]:

$$g^{off}_{nl} = z\,\frac{e^2}{h}\,\frac{\omega_c}{\omega_0^2}\sqrt{\omega_0^2+\omega_c^2}\sqrt{\frac{\hbar}{2\,m\,\omega_0}}\,\frac{m}{\hbar}\sum_{a,a'=0}^{\infty}\int_{-\infty}^{\infty} dE\left[-\frac{f(E+\hbar z)-f(E)}{\hbar z}\right]\times$$

$$\frac{\sqrt{a+1}}{\sqrt{\mathrm{k}^l_{-(a+1)}\,\mathrm{k}^l_{-a}}}\, e^{-i\,z\,\left(x/|v^n_{ga'}|+x_{\mathcal{A}}/|v^l_{ga+1}|\right)}\, e^{i\,\left(\mathrm{k}^l_{-(a+1)}-\mathrm{k}^l_{-a}\right)\,x_{\mathcal{A}}}\, S^*_{nl;a',a+1}(E+\hbar z)\, S_{nl,a'a}(E) \tag{17}$$

This contains further oscillatory exponentials, which for large $x_{\mathcal{A}}$ lead to suppression of the integral. However, this may be compensated by the fact that g_{nl}^{off} has roughly one power of wavenumber more than g_{nl}^{diag}. In that case the admittance at $B \neq 0$ can give information about products of S-matrix elements that cannot be written as a trace over subbands as in Eq. (1).

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[9] Experimentally, one may in fact be able to separate bulk and boundary contributions by varying a parameter such as the magnetic field in the leads, which may not significantly affect the internal $\Phi(\mathbf{x})$ in the sample area while causing observable changes in the external response, because the latter depends more sensitively on the *way* in which the carriers impinge on the sample region. This will be discussed in Ref. [10].

[10] J. U. Nöckel and K. Richter, unpublished